

1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate)

Safety Data Sheet 7H32714

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 04/27/2017

Revision date: 10/17/2018

Version: 1.1

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: 1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate)
CAS No	: 140681-55-6
Product code	: 7H32-7-14
Formula	: C7H14B2CIF9N2
Synonyms	: Selectfluor(TM); N-Fluoro-N'-chloromethyltriethylenediamine bis(tetrafluoroborate)
Other means of identification	: MFCD00142607

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture	: Laboratory chemicals Manufacture of substances Scientific research and development
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1.3. Details of the supplier of the safety data sheet

SynQuest Laboratories, Inc.
P.O. Box 309
Alachua, FL 32615 - United States of America
T (386) 462-0788 - F (386) 462-7097
info@synquestlabs.com - www.synquestlabs.com

1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

Classification (GHS-US)

Self-heat. 2	H252 - Self-heating in large quantities; may catch fire
Acute Tox. 4 (Oral)	H302 - Harmful if swallowed
Skin Irrit. 2	H315 - Causes skin irritation
Eye Dam. 1	H318 - Causes serious eye damage
Skin Sens. 1	H317 - May cause an allergic skin reaction
STOT SE 3	H335 - May cause respiratory irritation
Aquatic Acute 3	H402 - Harmful to aquatic life
Aquatic Chronic 3	H412 - Harmful to aquatic life with long lasting effects

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US)



Signal word (GHS-US)

: Danger

Hazard statements (GHS-US)

: H252 - Self-heating in large quantities; may catch fire
H302 - Harmful if swallowed
H315 - Causes skin irritation
H317 - May cause an allergic skin reaction
H318 - Causes serious eye damage
H335 - May cause respiratory irritation
H412 - Harmful to aquatic life with long lasting effects

Precautionary statements (GHS-US)

: P235+P410 - Keep cool. Protect from sunlight
P261 - Avoid breathing dust, mist, spray
P264 - Wash skin thoroughly after handling

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P270 - Do not eat, drink or smoke when using this product
P271 - Use only outdoors or in a well-ventilated area
P272 - Contaminated work clothing must not be allowed out of the workplace
P273 - Avoid release to the environment
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P301+P312 - If swallowed: Call a POISON CENTER or doctor/ physician if you feel unwell
P302+P352 - If on skin: Wash with plenty of soap and water
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310 - Immediately call a POISON CENTER or doctor/ physician
P321 - Specific treatment (see supplemental first aid instructions on this label)
P330 - Rinse mouth
P332+P313 - If skin irritation occurs: Get medical advice/attention
P333+P313 - If skin irritation or rash occurs: Get medical advice/attention
P362+P364 - Take off contaminated clothing and wash it before reuse
P363 - Wash contaminated clothing before reuse
P403+P233 - Store in a well-ventilated place. Keep container tightly closed
P405 - Store locked up
P407 - Maintain air gap between stacks/pallets
P413 - Store bulk masses greater than ...kg/...lbs at temperatures not exceeding ...°C/...°F
P420 - Store away from other materials
P501 - Dispose of contents/container to an approved waste disposal plant

2.3. Other hazards

No additional information available

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/information on ingredients

3.1. Substance

Substance type : Mono-constituent

Name	Product identifier	%	Classification (GHS-US)
1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate) (Main constituent)	(CAS No) 140681-55-6	<= 100	Self-heat. 2, H252 Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Dam. 1, H318 Skin Sens. 1, H317 STOT SE 3, H335 Aquatic Acute 3, H402 Aquatic Chronic 3, H412

Full text of H-phrases: see section 16

3.2. Mixture

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention.

First-aid measures after skin contact : Wash with plenty of soap and water. Remove contaminated clothing and shoes. In case of skin contact, wearing rubber gloves rub 2.5% calcium gluconate gel continuously into the affected area for 1.5 hours or until further medical care is available. Get immediate medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get immediate medical advice/attention.

First-aid measures after ingestion : Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/injuries : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

Symptoms/injuries after inhalation : Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

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4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Absorption of excessive F- can result in acute systemic fluorosis with hypocalcemia, interference with various metabolic functions and organ damage (heart, liver, kidneys).

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Thermal decomposition generates: Borane/boron oxides. Carbon oxides. Hydrogen fluoride. Nitrogen oxides.

5.3. Advice for firefighters

Firefighting instructions : In case of fire: Evacuate area.
Protection during firefighting : Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe dust.

6.1.1. For non-emergency personnel

Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Stop leak if safe to do so.
Methods for cleaning up : Sweep or shovel spills into appropriate container for disposal. Minimize generation of dust.
Other information : For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe dust, mist, spray. Wear personal protective equipment. Avoid contact with skin and eyes.
Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Comply with applicable regulations.
Storage conditions : Keep container closed when not in use. Moisture sensitive. Keep contents under inert gas.
Incompatible materials : Refer to Section 10 on Incompatible Materials.
Storage temperature : 2 - 8 °C Use explosion proof refrigerator
Storage area : Store in dry, cool, well-ventilated area.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

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8.2. Exposure controls

Appropriate engineering controls	: Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.
Hand protection	: Protective gloves. 29 CFR 1910.138: Hand Protection.
Eye protection	: Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection.
Skin and body protection	: Wear suitable protective clothing.
Respiratory protection	: In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection.
Other information	: Safety shoes. 29 CFR 1910.136: Foot Protection.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Color	: No data available
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: 260 °C
Freezing point	: No data available
Boiling point	: No data available
Flash point	: > 54 °C
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Vapor pressure	: No data available
Relative density	: No data available
Relative vapor density at 20 °C	: No data available
Molecular mass	: 354.26 g/mol
Solubility	: No data available
Log Pow	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

The product is stable at normal handling and storage conditions.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Keep away from heat, sparks and flame.

10.5. Incompatible materials

Strong oxidizing agents.

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10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed.

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ATE US (oral)	500.000 mg/kg body weight
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye damage.
Respiratory or skin sensitization	: May cause an allergic skin reaction.
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
Specific target organ toxicity (single exposure)	: May cause respiratory irritation.
Specific target organ toxicity (repeated exposure)	: Not classified
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: Absorption of excessive F- can result in acute systemic fluorosis with hypocalcemia, interference with various metabolic functions and organ damage (heart, liver, kidneys).
Symptoms/injuries after inhalation	: Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Waste treatment methods	: Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
Waste disposal recommendations	: Dispose of contents/container in accordance with licensed collector's sorting instructions.
Additional information	: Recycle the material as far as possible.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Transport document description : UN3088 Self-heating solid, organic, n.o.s., 4.2, II

UN-No.(DOT) : UN3088

Proper Shipping Name (DOT) : Self-heating solid, organic, n.o.s.

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Transport hazard class(es) (DOT) : 4.2 - Class 4.2 - Spontaneously combustible material 49 CFR 173.124
Hazard labels (DOT) : 4.2 - Spontaneously combustible



Packing group (DOT) : II - Medium Danger
DOT Packaging Non Bulk (49 CFR 173.xxx) : 212
DOT Packaging Bulk (49 CFR 173.xxx) : 241
DOT Symbols : G - Identifies PSN requiring a technical name
DOT Special Provisions (49 CFR 172.102) : IB6 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2). Additional Requirement: Composite IBCs 11HZ2 and 21HZ2 may not be used when the hazardous materials being transported may become liquid during transport.
IP2 - When IBCs other than metal or rigid plastics IBCs are used, they must be offered for transportation in a closed freight container or a closed transport vehicle.
T3 - 2.65 178.274(d)(2) Normal..... 178.275(d)(2)
TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.
DOT Packaging Exceptions (49 CFR 173.xxx) : None
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 15 kg
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 50 kg
DOT Vessel Stowage Location : C - The material must be stowed "on deck only" on a cargo vessel and on a passenger vessel.
Other information : No supplementary information available.

TDG

No additional information available

Transport by sea

UN-No. (IMDG) : 3088
Proper Shipping Name (IMDG) : SELF-HEATING SOLID, ORGANIC, N.O.S.
Class (IMDG) : 4.2 - Substances liable to spontaneous combustion
Packing group (IMDG) : II - substances presenting medium danger

Air transport

UN-No. (IATA) : 3088
Proper Shipping Name (IATA) : Self-heating solid, organic, n.o.s.
Class (IATA) : 4.2 - Substances Liable to Spontaneous Combustion
Packing group (IATA) : II - Medium Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate) (140681-55-6)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

EPA TSCA Regulatory Flag : P - P - indicates a commenced PMN substance.

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All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

This product or mixture does not contain a toxic chemical or chemicals in excess of the applicable de minimis concentration as specified in 40 CFR §372.38(a) subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR Part 372.

15.2. International regulations

CANADA

1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate) (140681-55-6)

Listed on the Canadian NDSL (Non-Domestic Substances List)

EU-Regulations

1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate) (140681-55-6)

Listed on ELINCS (European List of Notified Chemical Substances)

National regulations

1-Chloromethyl-4-fluoro-1,4-diazoniabicyclo[2,2,2]octane bis(tetrafluoroborate) (140681-55-6)

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

Listed on NZIoC (New Zealand Inventory of Chemicals)

Listed on the TCSI (Taiwan Chemical Substance Inventory)

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer and/or reproductive harm

SECTION 16: Other information

Revision date : 10/17/2018

Full text of H-phrases:

Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Aquatic Acute 3	Hazardous to the aquatic environment - Acute Hazard Category 3
Aquatic Chronic 3	Hazardous to the aquatic environment - Chronic Hazard Category 3
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Self-heat. 2	Self-heating substances and mixtures Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
Skin Sens. 1	Skin sensitization Category 1
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H252	Self-heating in large quantities; may catch fire
H302	Harmful if swallowed
H315	Causes skin irritation
H317	May cause an allergic skin reaction
H318	Causes serious eye damage
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H402	Harmful to aquatic life
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NFPA health hazard

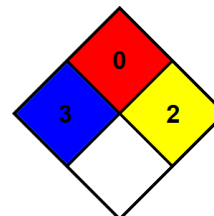
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

NFPA fire hazard

: 0 - Materials that will not burn.

NFPA reactivity

: 2 - Normally unstable and readily undergo violent decomposition but do not detonate. Also: may react violently with water or may form potentially explosive mixtures with water.



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HMIS III Rating

Health	: 2 Moderate Hazard - Temporary or minor injury may occur * - Chronic (long-term) health effects may result from repeated overexposure
Flammability	: 0 Minimal Hazard - Materials that will not burn
Physical	: 2 Moderate Hazard - Materials that are unstable and may undergo violent chemical changes at normal temperature and pressure with low risk for explosion. Materials may react violently with water or form peroxides upon exposure to air.

SDS US (GHS HazCom 2012)

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable or any damage resulting from handling or from contact with the above product.